

Scaling of electrical and thermal conductivities in an almost integrable chain

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Many low-dimensional materials are well described by integrable one-dimensional models such as the Hubbard model of electrons or the Heisenberg model of spins. However, the small perturbations to these models required to describe real materials are expected to have singular effects on transport quantities: integrable models often support dissipationless transport, while weak non-integrable terms lead to finite conductivities. We use matrix-product-state methods to obtain quantitative values of spin/electrical and thermal conductivities in an almost integrable gapless chain (an XXZ spin chain with staggered fields, or equivalently a spinless fermion chain with staggered on-site potentials). The results at low temperatures validate a scaling theory based on bosonization.

The physics of many one-dimensional systems with idealized interactions is rather special: the quantum Hamiltonian has infinitely many independent conserved quantities that are sums of local operators. Such Hamiltonians are called “integrable” in analogy with classical Hamiltonian systems that decompose into independent action and angle variables. Examples relevant to experiments on crystalline materials include the Hubbard model of electrons and the XXZ model of spins; ultracold atomic systems can realize integrable continuum models of bosons. However, in all these cases it is expected that integrability is only an approximation to reality and that experimental systems have integrability-breaking perturbations which, while small, drastically change some of the physical properties.

Transport of a conserved quantity such as charge, spin, or energy provides an experimentally important example of the effects of non-integrable perturbations. Integrable systems often have dissipationless transport or a “Drude weight” D in their frequency-dependent conductivity: [1–15]

$$\sigma(\omega) = 2\pi D\delta(\omega) + \dots, \quad (1)$$

where the ellipsis represents the nonsingular part of the conductivity. An experimental example of similar physics is the large, anisotropic thermal transport observed in $\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$ and attributed to a long mean free path of quasi-1D magnons [16–18]. We are interested here in the question of how the presence of generic integrability-breaking terms regularizes the zero-frequency conductivity [4–7, 12, 14, 19–23], as we expect many quasi-one-dimensional systems to be well described by integrable Hamiltonians plus weak non-integrable perturbations.

We apply a combination of numerical (matrix product states) methods to a suitable gapless non-integrable Hamiltonian to observe quantitatively the destruction of the thermal and electrical Drude weights. We compute the corresponding conductivities and analyze how they depend on temperature and the strength of the non-integrable perturbation. The results are compared to a scaling theory based on bosonization. One might expect

that on adding non-integrable terms, which generically destroy conserved quantities and hence the Drude weight, bosonization allows to obtain a parameter-free prediction for the conductivity at low temperature. By comparing with our numerics we obtain an understanding of the accuracy and range of validity of the bosonization approach.

We employ the XXZ chain in presence of a staggered magnetic field h which breaks integrability and focus on the parameter regime when this perturbation is irrelevant in the scaling sense and does not open a gap. We expect our key results (such as the scaling behavior of the conductivity at low temperatures) to hold for any gapless non-integrable model in which no conserved quantity protects the current. In the regime where h is relevant, its effects have been studied perturbatively [27, 28] and compared to experiments on spin diffusion in copper benzoate [29, 30]. A classic probe of quantum integrability, the absence of level repulsion in the energy spectrum, is used to show that this model is indeed non-integrable. We obtain numerical results for the electrical/spin and thermal conductivities using density matrix renormalization group (DMRG) methods which were developed in the past few years to access finite-temperature dynamics of correlated systems. Our model involves only nearest-neighbor interactions and can thus be studied efficiently via DMRG. By adapting previous bosonization techniques [8, 9] to the non-integrable perturbation in

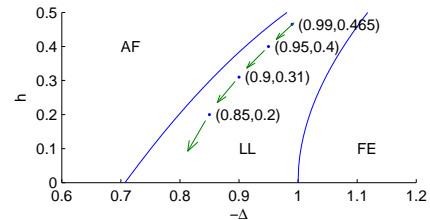


FIG. 1. The phase diagram [24, 25] of (2). The points share the same Luttinger liquid parameter $K \approx 2.4$ computed by DMRG [26].

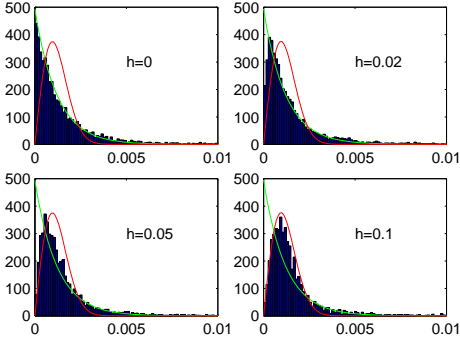


FIG. 2. The distributions of $\{E_{i+1} - E_i\}$, where $E_1 \leq E_2 \leq \dots \leq E_{4862}$ are the eigenenergies of (2) for $L = 18, \Delta = -0.8$ in the $S_z = 1, k = 2\pi/9$ sector (the total magnetization $S^z = \sum_{i=1}^L S_i^z$ and the momentum k are conserved). The green curve and red curve are best-fit exponential and Wigner-Dyson (orthogonal ensemble) distributions respectively. Neither the Poisson nor the Wigner-Dyson distribution appears clearly if we do not restrict to a symmetry sector of the model. The crossover to Wigner-Dyson with increasing h is observed independent of the choice of Δ and symmetry sector.

our model, we find testable predictions for the electrical conductivity at low temperature and compare them to the numerics.

The model. The XXZ model in a staggered magnetic field is given by $H = \sum_{i=1}^L h_i$ with

$$h_i = S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z + (-1)^i h S_i^z. \quad (2)$$

Without the staggered field, (2) is gapless for $|\Delta| \leq 1$ and gapped for $|\Delta| > 1$. Bosonization leads to the low-energy effective Hamiltonian for $|\Delta| \leq 1$ and infinitesimal h :

$$H = \frac{v}{2} \int dx \left(\Pi^2 + (\partial_x \phi)^2 \right) + ch \int dx \cos \left(2\sqrt{\pi K} \phi \right) + H_{\text{umklapp}} + H_{\text{band curv.}} + H_{\text{higher terms in } h}, \quad (3)$$

where Π is the conjugate momentum of the bosonic field ϕ with the canonical commutation relation $[\phi(x), \Pi(y)] = i\delta(x - y)$. The first term in (3) describes a Luttinger liquid. The Luttinger liquid parameter K is given through Bethe ansatz: $2K \arccos(-\Delta) = \pi$, and the coefficients v and c are also known exactly [31, 32]. As the scaling dimension of h is $2 - K$, the second term in (3) is relevant and opens a gap for $K < 2$ or $-\sqrt{2}/2 < \Delta \leq 1$; the term is irrelevant and (2) remains in the gapless Luttinger liquid phase for $K > 2$ or $-1 < \Delta < -\sqrt{2}/2$ (Fig. 1).

Integrability is well-defined in classical mechanics, but the definition of its quantum counterpart remains a subject of debate [33]. It is generally believed that the level spacing distribution (the distribution of the differences of the adjacent eigenenergies) is the exponential distribution for an integrable model, as levels appear as a Poisson

process, and the Wigner-Dyson distribution for a nonintegrable model. Intuitively, two nearby levels in an integrable model likely have different values of at least one integrable quantity, and thus live in different sectors of Hilbert space that are independent of each other; hence their energies are uncorrelated. Non-integrable models do not have an extensive number of such sectors and show energy level repulsion. The belief has been verified numerically on a variety of models [34, 35]. We perform an exact diagonalization of (2) with periodic boundary conditions. Fig. 2 shows the level spacing distributions, and the crossover from Poissonian behavior at $h = 0$ to the Wigner-Dyson distribution at nonzero h is clear. Hence (2) is nonintegrable for nonzero h .

Numerical approach. The DC charge (c) and heat (h) conductivities can be computed via the Kubo formula

$$\sigma = \lim_{t_M \rightarrow \infty} \lim_{L \rightarrow \infty} \frac{1}{LT} \text{Re} \int_0^{t_M} \langle J(t) J(0) \rangle dt, \quad (4)$$

where the corresponding current operators $J = \sum_{i=1}^L j_i$ are defined through a continuity equation [4]:

$$\begin{aligned} \partial_t h_i &= j_{h,i} - j_{h,i+1} \Rightarrow J_h = i \sum_{i=2}^L [h_{i-1}, h_i], \\ \partial_t S_i^z &= j_{c,i} - j_{c,i+1} \Rightarrow J_c = i \sum_{i=2}^L [h_{i-1}, S_i^z]. \end{aligned} \quad (5)$$

The current correlation functions $\langle J(t) J(0) \rangle$ can be computed efficiently using the real-time finite-temperature DMRG algorithm [36] introduced in [11]. DMRG is essentially controlled by the so-called discarded weight ϵ (we ensure that ϵ is chosen small enough and that L is chosen large enough to obtain numerically-exact results in the thermodynamic limit). The simulation is stopped when the DMRG block Hilbert space dimension χ reaches $\chi \sim 1000 - 1500$. This allows to access time scales $t \sim 10 - 20$ which are much larger than the inherent microscopic scale $t = 1$.

Results for $\langle J(t) J(0) \rangle$ are shown in Fig. 3. In the integrable case $h = 0$, the heat and charge Drude weights

$$D = \lim_{t \rightarrow \infty} \lim_{L \rightarrow \infty} \frac{\text{Re} \langle J(t) J(0) \rangle}{2LT} \quad (6)$$

are finite. A nonzero $h > 0$ renders the model nonintegrable; the current correlation functions decay to zero at large times, and the conductivities become finite. In order to compute the integral in Eq. (4) quantitatively, $\langle J(t) J(0) \rangle$ needs to be extrapolated. The heat current correlation function at intermediate to large temperatures $0.5 \leq T \leq \infty$ (see Fig. 3(b)) can be fitted by a single exponential function $\exp(-\lambda t)$ [37]. Oscillations develop at small T , but it is reasonable to assume that $\langle J(t) J(0) \rangle$ can be described by sums of exponentially decaying terms $\exp(-\lambda_n t + i\omega_n t)$ (the same holds for the

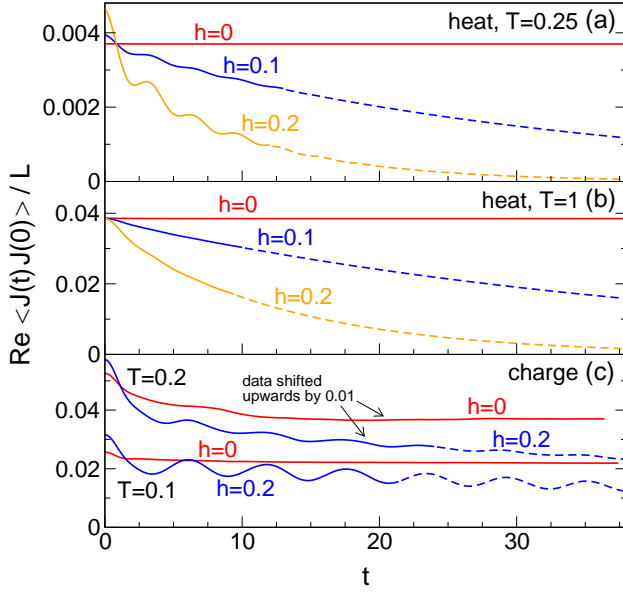


FIG. 3. Heat and charge current correlation functions $\langle J(t)J(0) \rangle$ at $\Delta = -0.85$. Their Fourier transform determines the corresponding conductivities through Eq. (4). The Drude weight (Eq. (6)) is nonzero only in the integrable case $h = 0$. A nonintegrable perturbation $h > 0$ renders the conductivity finite. DMRG data (solid lines) is extrapolated using linear prediction (dashed lines).

charge current correlation function). This motivates us to use so-called linear prediction [36] as an extrapolation procedure. Its stability can be tested by varying fit parameters (e.g. the number of terms or the fit interval) and by checking sum rules (see below); we can obtain accurate results for the heat conductivity at any h and temperatures $0.2 \lesssim T \leq \infty$ as well as for the charge conductivity at intermediate to large h and small $T \lesssim 0.3$.

Scaling of the conductivities: numerical results. DMRG data for the heat and charge conductivities is shown in Fig. 4. For fixed T and small h , one expects σ to diverge as [23]

$$\sigma \sim h^{-2} \text{ for } h \rightarrow 0. \quad (7)$$

This is confirmed by our results (for the thermal case see the inset to Fig. 4(a)). At small T , σ_c features power laws with nontrivial exponents:

$$\sigma_c \sim T^{\alpha_c} \text{ for } T \rightarrow 0. \quad (8)$$

Our model is a Luttinger liquid at low energies and one thus expects α_c to be a universal function of the Luttinger liquid parameter K only. This is verified in Fig. 4(b) which shows $\sigma_c(T)$ for different parameter sets (Δ, h) which share the same K (K can be determined from an independent ground state DMRG calculation [26]). The exponent $\alpha_c(K)$ varies strongly with K ; it is consistent with the analytic prediction $\alpha_c = 3 - 2K$ established below (see the insets to Fig. 4(b)). The heat conductivity

is only accessible for intermediate temperatures $T \gtrsim 0.2$; our data in this regime is almost independent of K (see Fig. 4(a)), suggesting that we have not reached the limit of low T .

Since for $h = 0$ the heat current is conserved by the Hamiltonian, the AC conductivity $\sigma_h(\omega, h = 0) = 2\pi D\delta(\omega)$ features a Drude peak only. By generalizing Eq. (4) to finite frequencies [8, 9], we can straightforwardly compute $\sigma_h(\omega, h)$ and demonstrate that it indeed becomes a δ -function series for $h \rightarrow 0$; the frequency-integrated heat conductivity just yields the Drude weight ('sum rule'). This is illustrated in Fig. 5 and provides an independent test for the reliability of our extrapolation procedure.

Scaling of the charge conductivity: theoretical analysis. We now present an analytic calculation of the low-temperature behavior of the charge conductivity σ_c assuming that the terms in Eq. (3) generated by h are already sufficient to destroy integrability. While this describes our data well, another possibility [20] is that integrability breaking results from the combination of h and umklapp, which leads to non-commuting $h \rightarrow 0$ and $T \rightarrow 0$ limits; this would also explain our data if we are currently in the small- h limit, but would predict a different behavior to set in at even lower temperatures. We start with a simple scaling analysis. Combining several simple assumptions, which are likely to hold for other 1D models, we establish a scaling form for the conductivity in which all the exponents are determined up to one number, the scaling dimension of the integrability-breaking perturbation. For our model, bosonization will verify this scaling ansatz and yield the scaling dimension.

Scaling analysis. It is reasonable to assume that $\text{Re}\langle J(t)J(0) \rangle / LT \approx A(\Delta, h, T) \exp(-\gamma(\Delta, h, T)t)$ at long time as correlations typically decay exponentially at finite T . The oscillation of this correlation function (see Fig. 3) of $\text{Re}\langle J(t)J(0) \rangle / LT$ is not taken into account, as it cancels out in computing the integral (4). We also assume the amplitude $A(\Delta, h, T)$ does not vanish as $T \rightarrow 0$ (note that the Drude weight $D(\Delta, h = 0, T)$ is nonzero and continuous as $T \rightarrow 0$). Then, (4) implies $\sigma_c \sim \gamma^{-1}$, and σ_c takes the scaling form

$$\sigma_c(\Delta, h, T) = f(\Delta/T^{[\Delta]}, h/T^{[h]})/T, \quad (9)$$

where $[\Delta]$ and $[h]$ are the scaling dimensions of Δ and h , respectively. Note that $\sigma_c \sim T^{-1}$ for $[\Delta] = [h] = 0$ or at the phase transition $\Delta = -\sqrt{2}/2, h = o(1)$.

In the perturbative regime (i.e., infinitesimal h), $[\Delta] = 0$ as there is no renormalization of Δ (it is exactly marginal). Then (9) simplifies to $\sigma_c(\Delta, h, T) = f(\Delta, h/T^{[h]})/T$. As one expects σ to diverge as h^{-2} by a golden-rule argument [23] unless this perturbation is inefficient in inducing scattering, we take $f(x) \sim x^{-2}$. Then

$$\sigma_c \sim h^{-2} T^{2[h]-1} = h^{-2} T^{3-2K} \quad (10)$$

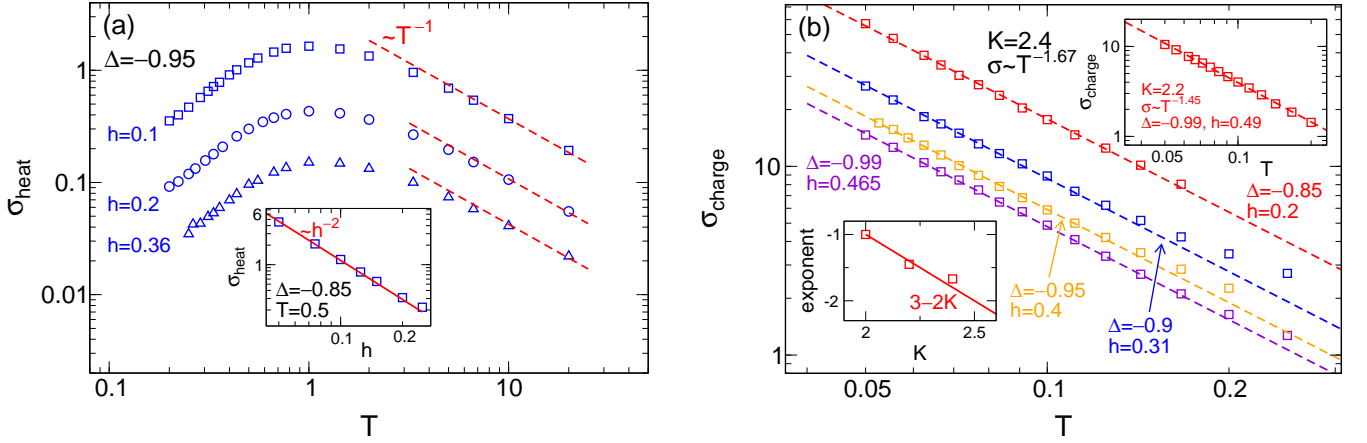


FIG. 4. Scaling of the heat and charge conductivities of a nonintegrable gapless spin chain. At low temperatures, $\sigma_c(T) \sim T^{\alpha_c(K)}$ is governed by power laws whose exponents are a universal function of the Luttinger liquid parameter K only. At fixed T , σ diverges as h^{-2} for $h \rightarrow 0$ with h being the strength of the nonintegrable perturbation [23]. Note that our definition of σ_h via Eq. (4) differs from the most common one [14] by a factor T^{-1} .

where in the second equality we have substituted the bosonization result $[h] = 2 - K$. Note that $\sigma_c \sim T^{-1}$ for $K = 2$ or at the phase transition $\Delta = -\sqrt{2}/2, h = o(1)$, consistent with the result at the end of the last paragraph.

The results of scaling for infinitesimal h will be reproduced by a perturbative field theory calculation using bosonization, which more convincingly justifies the assumptions in this section. However, it is worth pointing out that from the scaling analysis we still expect scaling of conductivity at low temperature in a gapless 1D system even when bosonization is inapplicable. In general a gapless 1D system with a single velocity of low-energy excitations will be described by a conformal field theory (CFT) at long distances, and such theories are effectively ballistic as left-moving and right-moving excitations decouple. We expect that the basic picture that conductivity is controlled by the leading irrelevant operator that induces scattering will still apply even when the CFT is more complicated than a free boson.

Bosonization. We now sketch a bosonization approach closely following Refs. 8 and 9 which studied transport in the integrable XXZ model. Note that in our case no conserved quantity protects the Drude weight. The current operator (5) reads $J_c = -v\sqrt{K/\pi} \int dx \Pi$, and the Kubo formula for the AC conductivity reduces to $\sigma_c(\omega) = iK\omega \langle \phi\phi \rangle_r(\omega)/\pi$. We perform a perturbative field theory calculation of the retarded correlation function $\langle \phi\phi \rangle_r$ to leading order in h , in H_{umklapp} , and in $H_{\text{band curv.}}$. The leading term governing the DC conductivity reads $\sigma_c = h^{-2}T^{3-2K}/C(K)$, which is consistent with Eq. (10) [38]. This term can be attributed to the staggered field, which is reasonable since the umklapp term alone does not destroy integrability and is thus less effective in scattering currents.

Outlook. Our work demonstrates an approach valid

for many actual 1D materials, in which integrability-breaking terms are likely to be present but small. We studied one specific model but expect that our key result – a power-law scaling of the conductivity $\sigma \sim T^\alpha$ with a universal exponent determined by the Luttinger liquid parameter – should be a general qualitative feature of any gapless nonintegrable model in which no conserved operator protects the current. Quantitative results for other nonintegrable perturbations can be obtained by the numerical framework used in this paper. It should be possible to compute optical charge conductivities for comparison to experiments on conducting polymers and other systems.

On a more basic level, quantum critical transport in one dimension is controlled by the leading irrelevant operators if and only if those destroy integrability. In higher

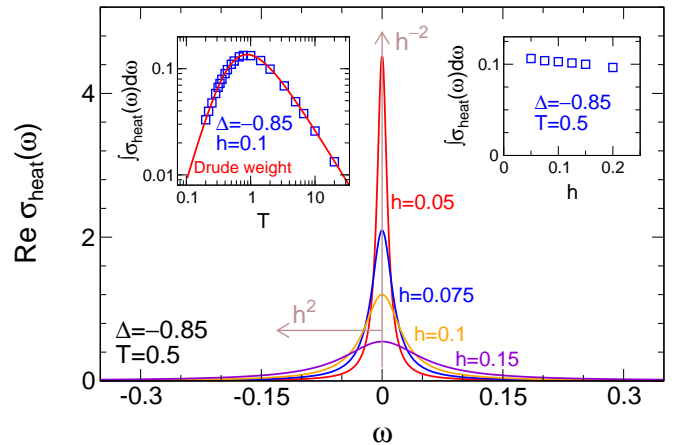


FIG. 5. AC heat conductivity. A Drude peak emerges as $h \rightarrow 0$: The integrated conductivity is independent of h (right inset) and equal to the Drude weight (left inset).

dimensions, quantum critical transport is different because the critical theory is believed to be non-integrable, and transport properties are actively being studied by methods from high-energy physics. Our results provide a constraint on these methods in a case where direct computation of transport coefficients is possible.

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- [37] An estimate of the Drude weight has been given for this model [39] under the assumption that thermal currents do not decay when $\hbar > 0$; as shown in Fig. 3, we find that thermal currents decay and the Drude weight is zero.
- [38] The prefactor can also be obtained easily: $C(K) = \pi^{K-3} (1 - K^{-1}/2)^{2K-1} \cos^2(\pi K/2) \sin^{1-2K}(\pi K^{-1}/2) \Gamma^2(K/2) \Gamma^2(1/2 - K/2) \Gamma^{2K} \left(\frac{1}{4K-2} \right) \Gamma^{-2K} \left(\frac{1}{2-K-1} \right) \exp \left(2 \int_0^{+\infty} \frac{dx}{x} \left(1 - (K-1)e^{-2x} - \frac{\sinh x}{\sinh((K^{-1}-1)x + \sinh x)} \right) \right)$; bosonization predicts $\sigma_c \approx 33$ at $\Delta = -0.85, h = 0.2, T = 0.05$, compared to the numerical result $\sigma_c \approx 57$ (Fig. 4). Noting that $h = 0.2$ is still not very small, the agreement is reasonable at all points in the regime $\Delta = -0.85, h = 0.2, T \lesssim 0.1$ and numerically we observe $\log \sigma_c / \partial \log h$ is slightly larger than -2 at $h = 0.2$, implying that the agreement is better at smaller h .
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